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Structure and vibrational spectra of mononitroalkanes

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Abstract

Structures and force fields for several mononitroalkane molecules were determined by ab initio quantum-chemical methods. The data obtained were used for calculation of the frequencies and modes of normal vibrations. Potentialities of different methods (RHF, MP2, and B3LYP) and basis sets for estimation of the structures and spectra were studied.

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Keywords

Force fields, Molecular structure, Mononitroalkanes, Quantum chemistry, Vibrational spectra